



LAWRENCE  
LIVERMORE  
NATIONAL  
LABORATORY

# X-Ray Diffraction and Raman Studies of Beryllium: Static and Elastic Properties at High Pressures

W. J. Evans, M. J. Lipp, H. Cynn, C. S. Yoo, M. Somayazulu, D. Hausermann, G. Shen, V. Prakapenka

April 28, 2005

Physical Review B

## **Disclaimer**

---

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

# **X-Ray Diffraction and Raman Studies of Beryllium: Static and Elastic Properties at High Pressures**

*W.J. Evans, M.J. Lipp, H. Cynn, C.S. Yoo*

H-Division, Physics and Advanced Technologies, Lawrence Livermore National  
Laboratory, Livermore, CA 94551, USA

*M. Somayazulu, D. Häusermann*

HPCAT, Argonne National Laboratory, Carnegie Institution of Washington, Advanced  
Photon Source, Building 434E, 9700 South Cass Ave., Argonne, IL 60439, USA

*G. Shen, V. Prakapenka*

GSECARS, CARS-The University of Chicago, Advanced Photon Source, Building  
434A, 9700 S. Cass Ave., Argonne, IL 60439, USA

## **Abstract**

We report combined x-ray and Raman studies of beryllium in helium or argon pressure medium at pressures approaching 200 GPa. Our results are generally consistent with recent studies confirming the stability of the hexagonal close-packed phase to the highest pressures. However, the quasi-hydrostatic conditions of our studies lead to a stiffer equation of state ( $K_0=109.88$ ,  $K_0'=3.59$ ) and a gradual approach toward a more ideal  $c/a$  ratio of 1.60 at 180 GPa. Combining our Raman and EOS data, we are able to evaluate the pressure dependence of the elastic shear modulus ( $C_{44}=109.3$ ,  $C'_{44}=1.959$ ). We discuss the comparison of our results with measurements using ultrasonic and dynamic techniques.

PACS number(s); 62.50.+p, 61.66.Bi, 64.30.+t, 63.20.-e

## **I. Introduction**

Beryllium is a unique metal with unusual properties of technological and scientific importance. Its physical properties are useful to the nuclear power industry as a neutron reflector/moderator and as a stiff lightweight structural element for aerospace structures. Further, beryllium exhibits an unusually high Debye temperature that leads to a large specific conductance and has thus been identified as a “hyperconductor” with favorable properties for efficient transmission of electrical power.<sup>1</sup> This combination of unique

properties and unusual behavior contribute to the characterization of beryllium as an “anomalous” metal. Scientifically beryllium has been the subject of a great deal of interest because of its simple atomic configuration and anomalous behavior. A simple atom with only two valence electrons (four total) would appear to be amenable to precise theoretical and *ab initio* modeling approaches. Contrary to this supposition, beryllium has been a difficult system to model and accurate theoretical predictions of its properties at high pressures have been elusive.<sup>2-5</sup> To address this broad interest, we have undertaken experimental studies of beryllium under high pressure conditions. Experimental studies of beryllium at high pressures measure the density dependence of fundamental properties, which will enable new applications and advance the basic scientific understanding of this material.

Beryllium at high pressure has been the subject of several experimental<sup>6-19</sup> and theoretical studies.<sup>2-5, 20-22</sup> At ambient conditions beryllium is a metal with a hexagonal close packed (hcp) crystal structure ( $\alpha$  phase) and a  $c/a$  ratio of 1.56,<sup>23</sup> far from the ideal value of 1.633. This non-ideal behavior is ascribed to the highly anisotropic bonding properties.<sup>3, 5</sup> At ambient pressure and high temperature beryllium transforms to a body centered cubic (bcc) crystal structure ( $\beta$  phase) at 1523 K, melts at 1551 K and finally boils at  $\sim 3243$  K.<sup>24</sup> At elevated pressure (up to 6 GPa) and high temperature, the  $\alpha$ - $\beta$  phase line has been observed to decrease with increasing pressure, with a negative slope of 45 K/GPa.<sup>8</sup> These data are summarized in the phase diagram shown in Fig. 1.

The  $\alpha$ - $\beta$  phase line (hcp-bcc) has been the source of continuing interest and controversy.<sup>6, 9, 17</sup> At ambient pressure, high-temperature experimental x-ray diffraction studies identified this hcp-bcc transition and measured an unusually large 4% decrease in specific volume.<sup>25</sup> At high pressures, the phase line was determined indirectly by monitoring the resistance of a beryllium sample in a belt-type large volume press.<sup>8</sup> A change in the resistance-vs-temperature slope was observed and used to identify the  $\alpha$ - $\beta$  phase line. Linearly extrapolating these data to room temperature, the phase line would be expected to cross 21 GPa at 300 K. It should be noted that there is some controversy regarding this observation.<sup>6</sup> Nevertheless, this negative slope stimulated several experimental and theoretical efforts to locate the continuation of this  $\alpha$ - $\beta$  phase line at room temperature. While several high-pressure electrical conductivity studies observed changes interpreted as the  $\alpha$ - $\beta$  transition,<sup>17, 26</sup> recent x-ray diffraction studies have found no such transitions.<sup>10, 16</sup> Theoretical efforts have found beryllium to be a challenging system, with predictions of the  $\alpha$ - $\beta$  phase line varying from 20 to 200 GPa.<sup>4, 5, 21, 27</sup> Thus previous studies have reported widely varying results.

Beryllium is a material with unique properties presenting both challenges and unique opportunities for experimental studies. As a low-Z element, beryllium has a very poor x-ray scattering efficiency, making diffraction measurements challenging. However, the light mass and hcp structure of beryllium lead to a single relatively high frequency Raman-active phonon mode (doubly degenerate  $E_{2g}$ ) that is suitable for Raman scattering measurements.

Recent studies of beryllium have addressed some of the controversial aspects of earlier work,<sup>10, 16</sup> but several questions remain. X-ray synchrotron studies of beryllium have established the stability of the hcp structure at room temperature to pressures approaching 200 GPa.<sup>10</sup> However, the experiments were performed without a hydrostatic pressure medium, so some question remains regarding the accuracy of the lattice

constants. Most importantly, the high stability of the hcp phase is in sharp contrast with the results of earlier low-pressure experiments<sup>8, 17, 26</sup> and theoretical predictions<sup>4, 5, 21</sup> and warrants confirmation. There has been one previous Raman spectroscopy study of beryllium at high pressure,<sup>12</sup> up to 30 GPa. In addition to static high-pressure studies of beryllium, there have been a few notable dynamic shock<sup>11, 19, 28, 29</sup> and isentropic compression experiments,<sup>14, 15, 18</sup> that complement static high pressure measurements and lead to the possibility of constructing a complete p-V-T equation of state.

In this report we present the results of studies using high-performance synchrotron sources to measure the crystal structure, lattice constants, and equation of state of beryllium to a pressure approaching 200 GPa (or 2.0 Mbar). Complementing the x-ray studies, we have measured the Raman spectrum of beryllium to pressures approaching 100 GPa. Combining both of these data, we evaluate the pressure-dependence of the elastic shear modulus,  $C_{44}$ . Finally, we discuss the implications of our work on the understanding of the properties of beryllium at high pressures.

## II. Experimental Procedure

The data presented in this report are the result of several x-ray diffraction and Raman spectroscopy experimental runs on beryllium using modern diamond anvil cell (DAC) techniques. We used Livermore-designed DACs of a modified Mao-Bell type and membrane-driven DACs. The anvils were 300  $\mu\text{m}$  flat diamonds and 300 $\mu\text{m}$  culet/100 $\mu\text{m}$  flat single-beveled diamonds for pressures below and above 50 GPa respectively. Rhenium gaskets were pre-indented to thicknesses of 20-40  $\mu\text{m}$  and drilled with sample chamber holes of 50-150  $\mu\text{m}$ . Beryllium samples were prepared by acid etching and rinsing a polycrystalline beryllium foil (Brush-Wellman, electro-refined 99.8% purity) to remove oxides and contaminants and carefully cutting a 20-50  $\mu\text{m}$  piece from the foil. The beryllium piece was loaded into the gasket hole along with a few micron-sized particles of gold (ruby) for *in-situ* pressure determination during the x-ray diffraction (Raman spectroscopy) run. We used hydrostatic pressure media in all of the experiments. In the case of x-ray diffraction, we used cryogenic techniques to load liquid helium, thereby minimizing diffraction signals from the pressure medium. Liquid argon was loaded cryogenically and served as the pressure medium in the cells designated for Raman spectroscopy.

X-ray diffraction was performed at both GSECARS and HPCAT beamlines of the Advanced Photon Source. X-ray spot sizes were  $\sim 20$   $\mu\text{m}$  and energies of 22 and 37 keV were used. The diffracted x-ray signal was detected using an image plate using exposure times of 5 minutes. The pressure was determined *in-situ* using the equation-of-state of the gold pressure marker.<sup>30</sup> The aperture in the diamond anvil cell limited the  $2\theta$ -scattering angle to  $\sim 25^\circ$ . The x-ray diffraction images consisted of uniform rings. Several diffraction peaks were observed below 100 GPa, including the (100), (002), (101), (102), (110) and (103). Above 100 GPa, the physical dimensions of the aperture in the DAC and the x-ray energy limited observed diffraction lines to the (100) and (101). Although these two lines are insufficient to make a structural determination, continuity with more complete spectra supports these peak identifications. Representative diffraction spectra are shown in Fig. 2. X-ray diffraction from the beryllium and gold pressure marker were measured simultaneously by selecting a spot on the sample where both materials were present. This approach minimized any possible systematic errors due

to pressure gradients and ensured accurate *in-situ* pressure measurements. Pressure determinations based on the accuracy of the gold diffraction peak determination were accurate to better than 0.5 GPa. Lattice constants of beryllium were measured to accuracies of better than 0.02% (for a) and 0.1% (for c).

Raman spectroscopy was performed using the 488 nm laser line of an argon ion laser. The laser was focused to a spot size of 15  $\mu\text{m}$  with an incident power level of less than 30 mW at the sample. The Raman scattered light was collected at an angle of  $\sim 30^\circ$  with respect to the incident laser beam. The Raman signal was spatially filtered and analyzed using a holographic notch filter, a 0.3 meter spectrograph, and a liquid-nitrogen-cooled CCD detector with an instrumental resolution of 0.24  $\text{cm}^{-1}$ . Typical exposure times were 5 minutes, gradually increasing to 30 minutes at our highest pressures near 100 GPa. The Raman phonon mode of beryllium was clearly evident, though more than  $5 \times 10^{-3}$  weaker than the diamond Raman signal. This weak signal is not inconsistent with the findings of previous polarized Raman studies of single crystals at ambient pressure. We observed no signal in the regime of the beryllium oxide phonon,<sup>31</sup> indicating a relatively pure sample with minimal oxide contamination. Pressure was determined *in-situ* using the ruby fluorescence technique,<sup>32</sup> with an accuracy of 0.5 GPa. Raman peaks were fitted and peak positions were determined with typical accuracies of 0.2  $\text{cm}^{-1}$ . At the pressures above 60 GPa, the weakening signal strength led to a gradual decrease in accuracy to 1.0  $\text{cm}^{-1}$ . The line width (FWHM) of the Raman mode increased approximately linearly with pressure from 7.97  $\text{cm}^{-1}$  at ambient pressure to 31.6  $\text{cm}^{-1}$  at 82 GPa. As with the x-ray diffraction, the pressure and Raman were collected from the same location without any repositioning to ensure that pressure gradients did not introduce systematic errors in the correlation of pressure to Raman spectrum. There was no observable pressure gradient across the sample chamber to within the accuracy of our pressure measurement. The Raman experiments ended not because of diamond anvil failure, but a gradual decrease in the Raman signal strength, probably due to the increasingly strong diamond background. A sampling of the collected Raman spectra is shown in Fig. 3.

### III. Analysis and Results

We present now the results of several experimental runs measuring x-ray diffraction and Raman spectra of beryllium under pressure. We were able to achieve pressures approaching 200 GPa and 100 GPa for x-ray diffraction and Raman spectroscopy respectively. Using a previously developed theoretical framework, we use these data to calculate the pressure-dependence of the elastic shear modulus of beryllium.

Beryllium was pressurized to a maximum pressure of 182 GPa. Consistent with previous studies,<sup>10</sup> beryllium remains in the hcp structure at room temperature and we find no evidence of any structural phase transitions. In Fig. 4a we present a graph of the isothermal equation of state at room temperature. For comparison data from other works are included. We fit our data to a third order Birch-Murnaghan equation, yielding parameters of 109.88(1.05) GPa and 3.584(0.027) for the bulk modulus and its pressure derivative respectively. Figure 4b shows the pressure dependence of the c/a ratio, which is initially flat, but above 60 GPa increases monotonically. Based on the accuracies stated above, the accuracy of the EOS and c/a ratio is dominated by the accuracy of our measurement of c and is thus  $\sim 0.1\%$ .

Our Raman studies extend up to 80 GPa, again showing no evidence of a phase transition and are in good agreement with the previous work of Olijnyk and Jephcoat at lower pressures.<sup>12</sup> We measured the Raman phonon energy to be 453.7 cm<sup>-1</sup> at ambient pressure. This differs somewhat with the measurement of Olijnyk (457 cm<sup>-1</sup>),<sup>12</sup> but is consistent with the studies of Feldman *et al.*<sup>33</sup> (455 cm<sup>-1</sup>). It is important to note that Olijnyk and Jephcoat used the 514.5 nm laser line for Raman excitation, while our studies and those of Feldman used the 488 nm line. This Raman energy dependence on excitation wavelength may be attributed to a strong phonon dispersion/probed wave vector effect, as noted by Ponosov *et al.* in the case of Osmium.<sup>34, 35</sup> Fig. 5 shows the pressure dependence of the Raman phonon line center. The pressure dependence is approximately linear in pressure with a slight decrease in slope with increasing pressure. We fit the data to a second order polynomial in pressure (units of GPa) with coefficients 459(2.1), 2.806(0.113) and -0.011(0.001).

Using the collected data, we have calculated the elastic shear modulus of beryllium. The Raman phonon mode being measured represents a collective excitation where adjacent hexagonal planes of atoms oscillate against each other. Thus it is reasonable to expect that the Raman phonon reflects the behavior of the elastic shear modulus,  $C_{44}$ . An expression for the elastic shear modulus has been derived for the hcp structure with the assumption of isotropic interaction potentials.<sup>12, 36-40</sup> The expression describing this relationship, as given by Olijnyk, is:

$$v_{TO}(k=0) = \sqrt{\frac{\sqrt{3}a^2C_{44}}{\pi^2mc}}$$

Using the result of our EOS fit to the beryllium p-V data, we apply this expression and calculate the elastic shear modulus,  $C_{44}$ . The results of this calculation are shown in Fig. 6. Propagating the errors in the parameters, the accuracy of our determination of  $C_{44}$  is approximately 1%. Our results are in good agreement with the work of Olijnyk<sup>12</sup> and extend the experimentally measured range of the dependence to pressures approaching 100 GPa. A quadratic fit to the data points versus pressure yields the parameters 110.6(1.0), 1.784 (0.056), and -0.0028 (0.0007) for the y-intercept, slope and second derivative, respectively. The small second derivative demonstrates that the relation is generally linear over this pressure range.

#### IV. Discussion

Our x-ray diffraction studies yield an isothermal EOS that differs noticeably from previous studies. Our measured EOS is substantially stiffer than the EOS of Nakano *et al.*<sup>10</sup> This is clearly evident in Fig. 4, amounting to a 2-4 % difference in volume at pressures above 100 GPa. The cause of this difference is not clear, but could possibly be due to systematic effects in determining the pressure in a non-hydrostatic sample with a pressure gradient. We tentatively ascribe the difference to the use of a hydrostatic medium, helium, whereas the previous studies used no medium. We note that our results agree quite well with the work of Velisavljevic *et al.*,<sup>16</sup> where a copper pressure-calibrant/medium was used up to a pressure of 66 GPa. More generally our bulk modulus and its derivative are in reasonable agreement with dynamic measurements shown in

table 1 (the bulk modulus for the shock measurement was determined by fitting a Birch-Murnaghan function to the  $T=0$  isotherm that had been deduced from the shock data<sup>28</sup>). The static isothermal  $pV$ -data we present here may be combined with detailed analysis of recent dynamic measurements<sup>11, 15, 18, 19</sup> to construct an experimentally-validated complete  $pVT$ -EOS.

An important finding of our work is the increase of the  $c/a$  ratio from 1.56 at ambient pressure to 1.60 at 180 GPa. The increase in  $c/a$  occurs at pressures above 50 GPa, just beyond the range of previous work that observed no significant variation.<sup>16</sup> The deviation of the  $c/a$  ratio of beryllium at ambient pressure is ascribed to anisotropic bonding, namely a strongly covalent bond character, with a component aligned along the  $c$ -axis.<sup>5</sup> The gradual increase in  $c/a$  observed in our studies suggests an increasingly isotropic interatomic potential. This change is important because it serves to justify our use of the model described above for the elastic shear modulus of beryllium. In particular, the model was developed assuming an isotropic force potential. Thus, because our EOS measurements imply an isotropic potential, we expect our evaluation of  $C_{44}$  to be increasingly valid at higher pressures. For the purpose of validating theoretical modeling efforts, one would expect credible approaches to reproduce not only the  $pV$  data but also the change in  $c/a$ . We further note that recent studies suggest that such an abrupt shift in the  $c/a$  dependence may be the result of Lifshitz electronic transition.<sup>41</sup> Ocelli *et al.* identified a subtle discontinuity in the slope of the  $c/a$  pressure-dependence of osmium and associate this with an electronic anomaly. Although there are conflicting measurements<sup>42</sup> of osmium regarding the presence of this discontinuity, in the case of beryllium we find an abrupt clearly identifiable change in slope at  $\sim 50$  GPa. Within the context of the proposed Lifshitz transition, our measurements of beryllium present a compelling case for further theoretical and experimental study.

Our evaluation of  $C_{44}$  differs markedly from ambient pressure ultrasonic measurements,<sup>43, 44</sup> but is consistent with the work of Olijnyk and Jephcoat,<sup>12</sup> as shown in table 1. The anisotropic bonding of beryllium at low pressures is a possible explanation for the observed deviation between our evaluation and the results of ultrasonic measurements. Namely, the model we have used is not entirely appropriate for the low-pressure anisotropic bonding, however it will become increasingly valid as the pressure and thus  $c/a$  ratio approaches a value consistent with an isotropic potential. Thus despite the limitations of the model, we believe our evaluation of  $C_{44}$  to be increasingly accurate at higher pressures.

#### IV. Conclusion

In summary, we have measured the room temperature lattice constants and Raman phonon of beryllium under hydrostatic conditions up to pressures of 180 GPa and 80 GPa respectively. We determine the bulk modulus and its derivative to be 109.88 and 3.584. The  $c/a$  ratio increases with pressure achieving 1.60 at 180 GPa. The Raman phonon shifts linearly with pressure, fitting to a line with an initial value of  $459 \text{ cm}^{-1}$  and a slope of  $2.806 \text{ cm}^{-1}/\text{GPa}$ . Finally we used our data to evaluate the elastic shear modulus, which fits to a line beginning at 110.6 GPa and a slope of 1.784. Although we find qualitative agreement with previous studies, our measured EOS is stiffer than non-hydrostatic

studies. Our Raman studies increase the measured pressure range by more than a factor of two, and permit the evaluation of the elastic shear modulus to pressures approaching 100 GPa. We do not observe any phase transitions at room temperature. These data should be valuable in modeling of beryllium under pressure and developing a complete pVT EOS model of this technologically important material.

### **Acknowledgements**

This work was performed under the auspices of the U.S. DOE by the Univ. of Calif., LLNL under contract No. W-7405-Eng-48. Work performed at HPCAT was supported by DOE-BES, DOE-NNSA, NSF, DOD-TACOM, and the W.M. Keck Foundation and at GeoSoilEnviroCARS, by the NSF- Earth Sciences (EAR-0217473), DOE-Geosciences (DE-FG02-94ER14466) and the State of Ill. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38. The authors acknowledge use of the program FIT2D developed by A. Hammersley of ESRF. We thank Sam Weir for useful discussions.

## References

- 1 F. M. Mueller, K. A. Johnson, W. J. Medina, et al., Applied Physics Letters **57**,  
240 (1990).
- 2 M. Y. Chou, P. K. Lam, and M. L. Cohen, Solid State Communications **vol.42**,  
**no.12**, 861 (1982).
- 3 M. Y. Chou, P. K. Lam, and M. L. Cohen, Physical Review B (Condensed  
Matter) **vol.28**, **no.8**, 4179 (1983).
- 4 P. K. Lam, M. Y. Chou, and M. L. Cohen, Journal of Physics C (Solid State  
Physics) **vol.17**, **no.12**, 2065 (1984).
- 5 A. K. McMahan, AIP Conference Proceedings **no.78**, 340 (1981).
- 6 A. Abey, (Lawrence Livermore National Laboratory, Livermore, CA, 1984), p.  
13.
- 7 A. E. Abey and R. L. Reichlin, Bulletin of the American Physical Society **26**, 667  
(1981).
- 8 M. Francois and M. Contre, in *Conference Internationale sur la Metallurgie du*  
*Beryllium* (Universite de France, Paris, Grenoble, 1965).
- 9 L. C. Ming and M. H. Manghnani, Journal of Physics F (Metal Physics) **vol.14**,  
**no.1**, L1 (1984).
- 10 K. Nakano, Y. Akahama, and H. Kawamura, Journal of Physics: Condensed  
Matter **vol.14**, **no.44**, 10569 (2002).
- 11 W. J. Nellis, J. A. Moriarty, A. C. Mitchell, et al., Journal of Applied Physics  
**vol.82**, **no.5**, 2225 (1997).
- 12 H. Olijnyk and A. P. Jephcoat, Journal of Physics-Condensed Matter **12**, 8913  
(2000).
- 13 R. L. Reichlin, Review of Scientific Instruments **54**, 1674 (1983).
- 14 D. C. Swift, D. L. Paisley, G. A. Kyrala, et al., AIP Conference Proceedings  
**no.620**, **pt.2**, 1192 (2002).
- 15 D. Swift, D. Paisley, and M. Knudson, AIP Conference Proceedings **no.706**, **pt.1**,  
119 (2004).
- 16 N. Velisavljevic, G. N. Chesnut, Y. K. Vohra, et al., Physical Review B **65**  
(2002).
- 17 V. Vijayakumar, B. K. Godwal, Y. K. Vohra, et al., Journal of Physics F (Metal  
Physics) **vol.14**, **no.5**, L65 (1984).
- 18 D. B. Reisman, A. Toor, R. C. Cauble, et al., Journal of Applied Physics **vol.89**,  
**no.3**, 1625 (2001).
- 19 R. Cauble, T. S. Perry, D. R. Bach, et al., Physical Review Letters **80**, 1248  
(1998).
- 20 H. C. Graboske, R. Grover, and K. Long, Bulletin Of The American Physical  
Society **24**, 724 (1979).
- 21 B. Palanivel, R. S. Rao, B. K. Godwal, et al., Journal of Physics: Condensed  
Matter **vol.12**, **no.41**, 8831 (2000).
- 22 D. A. Young, *Phase diagrams of the elements* (University of California Press,  
Berkeley, 1991).
- 23 J. Donohue, *The structures of the elements* (Wiley, New York, 1974).
- 24 J. Elmsley, *The Elements* (Oxford University Press, London, 1998).
- 25 A. J. Martin and A. Moore, Journal of the Less Common Metals **1**, 85 (1959).

- 26 A. R. Marder, *Science* **142**, 664 (1963).
- 27 J. C. Boettger, *International Journal Of Quantum Chemistry* **56**, 197 (1995).
- 28 R. G. McQueen, S. P. Marsh, J. W. Taylor, et al., in *High-Velocity Impact Phenomena*, edited by R. Kinslow (Academic Press, New York, 1970).
- 29 J. L. Wise, L. C. Chhabildas, and J. R. Asay, *AIP Conference Proceedings* **78**, 417 (1982).
- 30 O. L. Anderson, D. G. Isaak, and S. Yamamoto, *Journal Of Applied Physics* **65**, 1534 (1989).
- 31 A. P. Jephcoat, R. J. Hemley, H. K. Mao, et al., *Physical Review B (Condensed Matter)* **vol.37, no.9**, 4727 (1988).
- 32 H. K. Mao, J. Xu, and P. M. Bell, *J. Geophys. Res.* **91**, 4673 (1986).
- 33 D. W. Feldman, J. H. Parker, Jr., and M. Ashkin, *Physical Review Letters* **vol.21, no.9**, 607 (1968).
- 34 Y. S. Ponosov, G. A. Bolotin, C. Thomsen, et al., *Physica Status Solidi B-Basic Research* **208**, 257 (1998).
- 35 Y. S. Ponosov, I. Loa, V. E. Mogilenskikh, et al., *arXiv.org* **cond-mat/0503272** (2005).
- 36 E. A. Metzbower, *Phys. Status Solidi* **25**, 403 (1968).
- 37 H. Olijnyk and A. P. Jephcoat, *Solid State Communications* **115**, 335 (2000).
- 38 H. Olijnyk and A. P. Jephcoat, *High Pressure Research* **22**, 43 (2002).
- 39 H. Olijnyk and A. P. Jephcoat, *Metallurgical and Materials Transactions a-Physical Metallurgy and Materials Science* **33**, 743 (2002).
- 40 J. C. Upadhyaya, D. K. Sharma, D. Prakash, et al., *Canadian Journal of Physics* **72**, 61 (1994).
- 41 F. Occelli, D. L. Farber, J. Badro, et al., *Physical Review Letters* **93** (2004).
- 42 T. Kenichi, *Physical Review B* **70** (2004).
- 43 W. D. Rowland and J. S. White, *Journal of Physics F (Metal Physics)* **2**, 231 (1972).
- 44 D. J. Silversmith and B. L. Averbach, *Physical Review B (Solid State)* **vol.1, no.2**, 567 (1970).

## Figure Captions

FIG 1. Phase diagram of beryllium. High pressure data of Francois and Contre<sup>8</sup> establishing the hcp, bcc and liquid phase lines is shown.

FIG 2. Representative x-ray diffraction patterns over the pressure range covered in this report. 2a and 2b are at x-ray photon wavelengths of 0.3311 Å, and 0.5659 Å respectively. Pressures are indicated adjacent to trace. Peaks due to the rhenium gasket and gold pressure marker are marked with an asterisk(\*) and dagger(†) respectively.

FIG 3. Representative Raman spectra spanning the pressure range covered in this report. Pressure are indicated adjacent to spectra. Spectra are scaled and shifted for clarity.

FIG 4. Equation of state and c/a ratio of beryllium measured in this work (open circles). For comparison, the measurements of Nakano et al.<sup>10</sup> (open squares) are shown. Upper panel shows unit cell volume as a function of pressure. Lower panel shows the change in the c/a ratio with pressure.

FIG 5. Pressure dependence of the Raman shift of the TO phonon in Beryllium. Circles are this work and squares are the work of Olijnyk and Jephcoat<sup>12</sup> The straight line is a 2<sup>nd</sup> order polynomial fit to our data,  $E(\text{in cm}^{-1})=459 + 2.806 P (\text{in GPa}) - 0.011 P^2$ .

FIG 6. Pressure dependence of the elastic shear modulus of beryllium. Circles are calculations using our data, and the line is a 2<sup>nd</sup> order polynomial fit,  $C_{44}(\text{in GPa})= 110.6 + 1.784 P (\text{in GPa}) - 0.0028 P^2$ .

## Table Captions

Table 1. Comparison of bulk modulus and its derivative for static and dynamic measurements.

Table 2. Comparison of  $C_{44}$  evaluation.

**Figures**

Figure 1

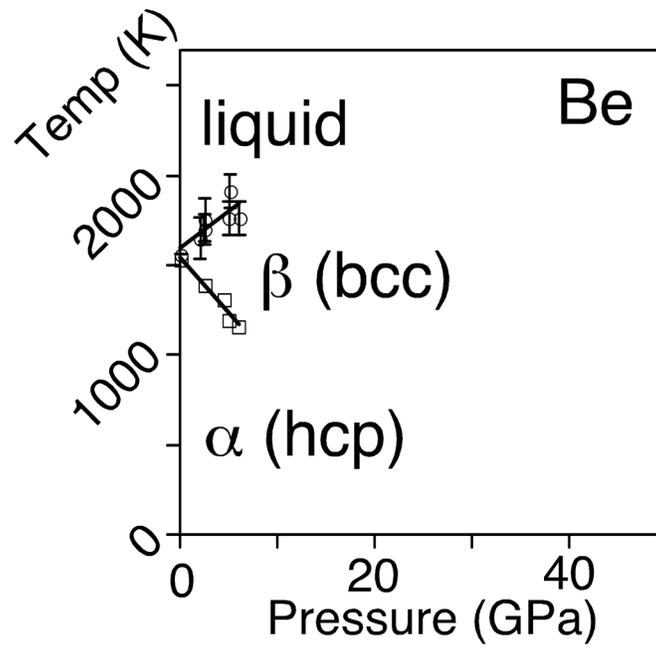


Figure 2

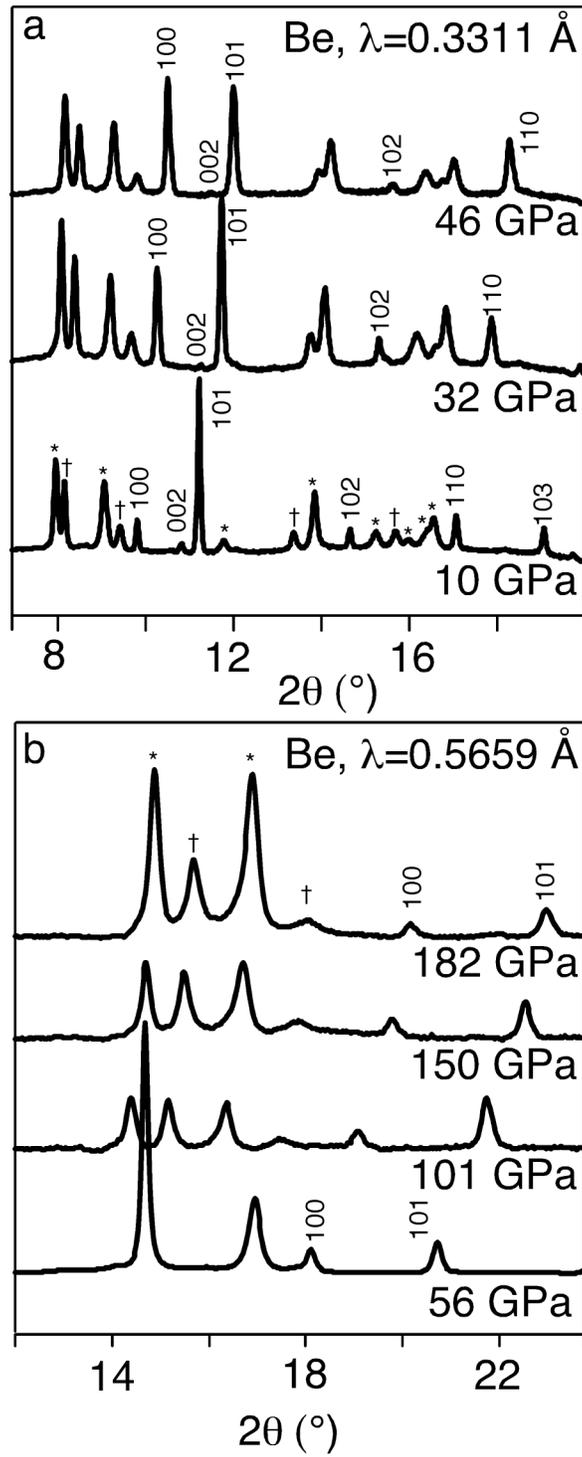


Figure 3

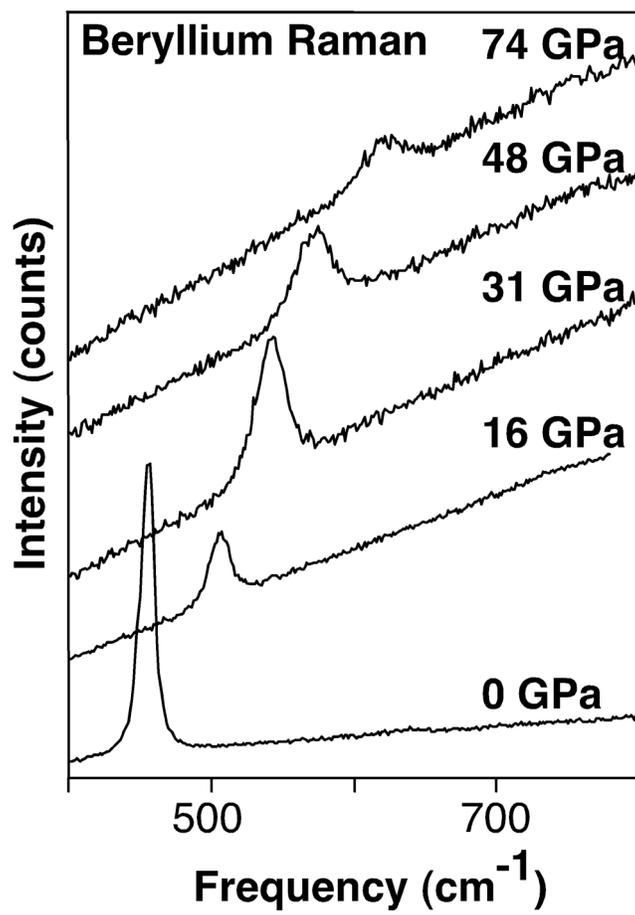


Figure 4

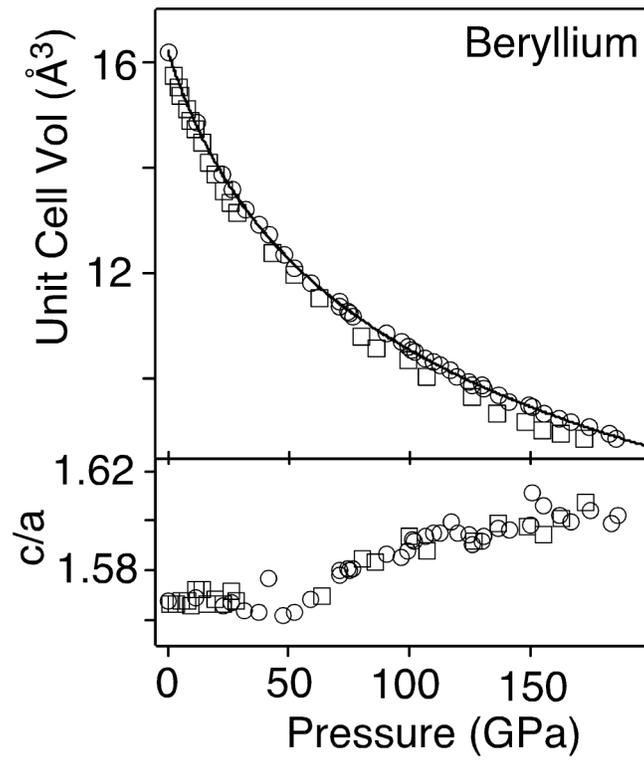


Figure 5

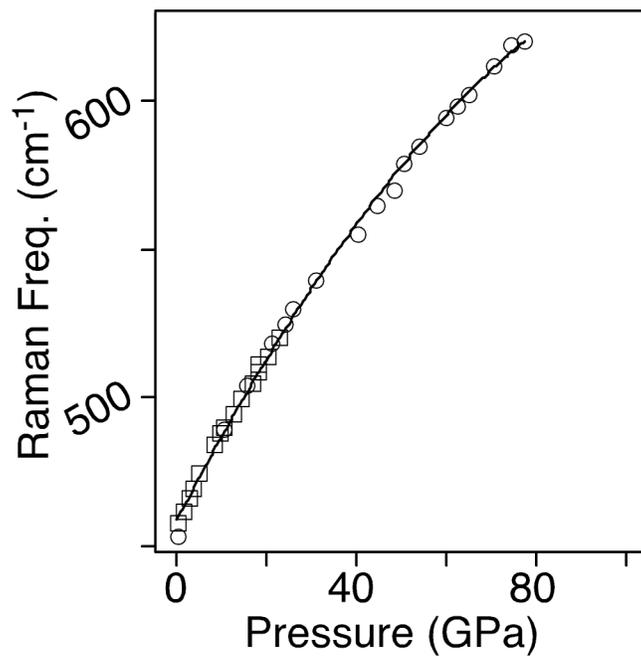
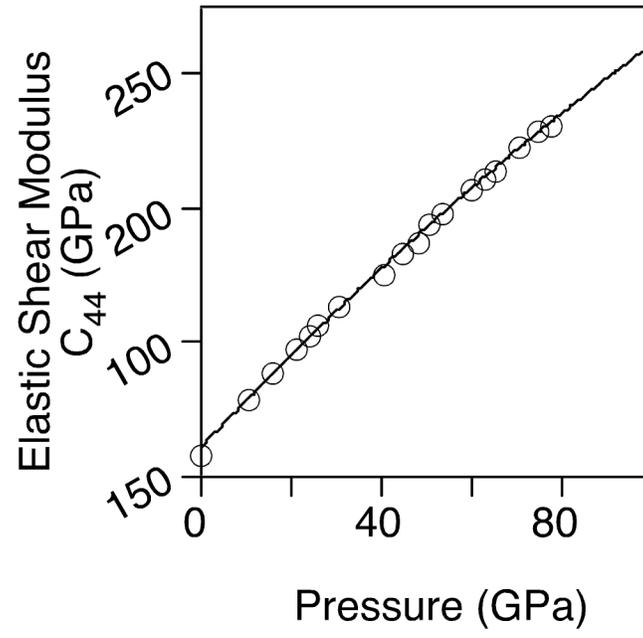


Figure 6



## Tables

Table 1

Technique	$K_0$	$K'_0$
DAC (This work)	109.88 (1.05)	3.59 (0.03)
DAC <sup>10</sup>	97.2 (2.5)	3.61 (0.007)
DAC <sup>16</sup>	106.5	3.541
Shock <sup>28</sup>	114.97	3.55

Table 2

Technique	$C_{44}$ (GPa)	$C'_{44}$
DAC (This work)	110.6 (1.0)	1.78(0.06)
DAC <sup>12</sup>	110	1.65
Ultrasonic <sup>43</sup>	154.9	
Ultrasonic <sup>44</sup>	170.6	2.55